

AFML-TR-67-121

PART VII

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EVALUATION OF MOLECULAR WEIGHT FROM EQUILIBRIUM SEDIMENTATION

PART VII MATHEMATICAL ANALYSIS OF THE REGULARIZATION
TECHNIQUE INCORPORATED INTO QUADRATIC PROGRAMING

DONALD R. WIFF
MATATIAHU T. GEHATIA
THOMAS E. DUVALL

TECHNICAL REPORT AFML-TR-67-121, PART VII

DECEMBER 1972

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AFML-TR-67-121

PART VII

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FOREWORD

This report was prepared by the Polymer Branch of the Nonmetallic Materials Division. The work was initiated under Project No. 7342, "Fundamental Research on Macromolecular Materials and Lubrication Phenomena," Task No. 734203, "Fundamental Principles Determining the Behavior of Macromolecules," Subtask No. 734203-05, "Physical Chemistry of High Polymers", with Dr. M. T. Gehatia acting as subtask scientist. Coauthors are Mr. T. E. Duvall, ASD Computer Science Center (4950/VNCS), and Dr. D. R. Wiff, Research Institute, University of Dayton. The work was administered under the direction of the Air Force Materials Laboratory, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio.

The report covers research conducted from September 1971 to May 1972. The manuscript was released by the authors in June 1972 for publication as a technical report.

This technical report has been reviewed and is approved.



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ABSTRACT

The equation relating molecular weight distribution of a polymer to the experimental function of concentration appearing in equilibrium sedimentation with the ultracentrifuge is nonsolvable because it is an Improperly Posed Problem in the Hadamard sense. For a simple distribution this equation has been solved by applying a method of regularization. To solve a nonsymmetrical bimodal and a trimodal distribution, the technique of regularization had to be incorporated into a linear programming. In the current work the regularization technique has been incorporated into quadratic programming. This new combined method proved to be more adequate to solve, also more complex distributions such as tri-, tetra-, and pentamodal. In addition this technique is cheaper, because it requires less computer time than the regularization incorporated into linear programming.

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SECTION I

INTRODUCTION

The increased use of polymeric materials by the U.S. Air Force has placed an ever increasing demand upon the reliability e. g., strength, of these materials. Many bulk property characteristics: density, shear modulus, stress modulus, high temperature resistance, tenacity, etc. are dependent upon the distribution of molecular weights of the macromolecular chains composing the material.

There are many interacting morphological patterns - tie molecules, degrees of crystallinity, varying degrees of order-which manifest various bonding energies and/or intra-molecular interactions. These affect the strength of a polymeric material in the bulk state. However, if the molecular weight is too low, the strength can be affected as a result of pure thermal (Brownian) motion. An extremely high molecular weight might, on the other hand, inhibit relaxation or even hinder the processability of the material. If molecular weight affects the final bulk state properties to such a degree, a distribution of molecular weights adds another variable that can greatly affect the reliability of these materials.

For these reasons, a mathematical procedure for obtaining a molecular weight distribution (MWD) from equilibrium sedimentation data was necessary.

There exist differential and integral equations describing important physical or technological systems which in general cannot be solved by usual mathematical means and even by approximation because they belong to the class of improperly posed problems (IPP). To this class also belongs the equation which relates MWD to the concentration function provided by the technique of equilibrium sedimentation.

The notion of an IPP (improperly posed problem or incorrectly formulated problem) goes back to Hadamard (Reference 1) in conjunction

with the Cauchy problems of potential and a number of inverse problems for differential and integral equations. In the recent decade IPP's have been intensively investigated. The following considerations with respect to ill-posedness of a mathematical problem and the ways leading to their solution is based on the ideas of Phillips (Reference 2), John (References 3, 4), Lavrentiev (Reference 5), Tikhonov (References 6-21), Ivanov (References 22-26), and others (References 27-42). Among the class of IPP there exists a subclass of regularizable IPP which can be solved by applying a method of regularization.

To the subclass of regularizable IPP also belong the equation mentioned before associated with MWD determination via equilibrium sedimentation. Because of the need to correlate a MWD with physical and mechanical properties of synthetic polymers an attempt has been made in this laboratory to solve this particular equation. The progress of this work has been described in a series of technical reports AFML-TR-67-121, Parts I through VI. The first attempts to derive an MWD from these equations without using the regularization technique were unsatisfactory (Parts I through III). In part IV regularization was successfully applied and good results were obtained in case of a unimodal distribution. To solve more complex distributions, such as symmetrical and asymmetrical bimodal and symmetrical trimodal, regularization was incorporated into a linear programming algorithm (Part V). In Part VI this method was experimentally verified. An artificial and a priori known distribution of polystyrene samples was investigated. The resulting distribution was in very good agreement with the one artificially prepared.

This regularization - linear programming technique seemed limited to a maximum trimodal multiplicity. In addition, a large amount of valuable digital computer time was consumed in search for appropriate regularizing parameters.

Therefore the present report (Part VII) extends the previously discussed modifications to include regularization into quadratic programming. The required computation time is greatly diminished and the

multiplicity capable of being resolved now includes a tetramodal MWD. This paper is divided into sections, such that, once the mathematical definition of an ill-posed problem is, specified, the technique of regularization used later in the discussion, will be explained. This technique leads to better results if it is incorporated in the quadratic programming. However, before discussing this latest refined combination of methods, a brief discussion of a quadratic programming technique follows. Then the actual Fredholm Integral of the First Kind used along with examples of its ill-posedness is illustrated. Finally, the incorporation of regularization into quadratic programming with its application to a specific kernel will be presented.

The preceding AFML-TR-67-121 reports previously referred are:

- Part I , M. T. Gehatia (June 1967).
- Part II , M. T. Gehatia and D. R. Wiff (April 1969).
- Part III, R. R. Jurick, D. R. Wiff and M. T. Gehatia (May 1970).
- Part IV , M. T. Gehatia and D. R. Wiff (August 1970).
- Part V , D. R. Wiff and M. T. Gehatia (February 1971).
- Part VI , M. T. Gehatia and D. R. Wiff (November 1971).

SECTION II

ILL-POSED PROBLEM AND REGULARIZATION

Let F and U be some complete metric spaces. Let Af be a function with domain of definition F and the range of values U . Consider the equation

$$Af = U = Q [\xi, f(m)] \quad (1)$$

The problem of solving Equation 1 for a set $\{f\}$ given a set $\{u\}$ and knowing the functional form of A is a properly posed problem if the following conditions are satisfied:

- (1a) The solution of Equation 1 exists for any $u \in U$.
- (1b) The solution of Equation 1 is unique in F .
- (1c) The solution of Equation 1 depends continuously on u in the metrics of F and U . In such a case there exists a function Ou defined and continuous over all U , and O is an inverse operator of A , where

$$Ou = A^{-1} u = f = R [m, u(\xi)] \quad (2)$$

If even one of the conditions (1a), (1b) or (1c) is not satisfied $[u = Af]$ is an IPP. In such a case the function O either does not exist or it is not stable and not reliable. Many expressions of mathematical physics include linear operations. In this case U and F are Banach Spaces and A is a linear operator. The Banach Spaces U and F encountered in most cases are the known functional spaces C^l , L_p , W_p^b , H_p^q , S_p , . . . with the carriers in some n -dimensional space of the independent variables or on any part of the spaces of independent variables. The first requirement of correctness is that the problem under consideration should not be overdetermined; second that the solution is unique, since the right-hand side of Equation 1 are real quantities obtained by measurements;

and the third condition requires the continuity of the inverse function Ou . It was felt for a long time that if at any point u the function Ou was discontinuous, then the solution f could not be uniquely recovered from the right hand side u . Hadamard introduced the notion of well-posedness by giving an example of an IPP which became a classical textbook example. This example was the famous Cauchy problem for the Laplace equation. Hadamard did not believe that an IPP represents any real physical system. This later conclusion proved to be erroneous, and many real equations of mathematical physics lead to problems which are improperly posed in the sense of Hadamard.

We now formulate an approach to the question of well-posedness of problems of the type under consideration. The approach consists of changing the notion of correctness by having requirements different from (1a), (1b), and (1c) above. In addition to the spaces U and F and the operator A , let there be given some closed set $\Phi \subset U$. According to Tikhonov, the solution of Equation 1 is properly posed if

(2a) It is "a priori" known that the solution f exists for some class of data and belongs to the given set Φ , $f \in \Phi$.

(2b) The solution is unique in a class of functions belonging to Φ .

(2c) Arbitrarily small changes in u do not carry the solution f out of Φ corresponding to arbitrarily small changes in the solution f .

Upon denoting Φ_A the image of Φ after the application to the space F of the operator A , requirement (2c)₁ can be restated as

(2c)₂ The solution of Equation 1 depends continuously on the right-hand side of u on the set Φ_A .

If Φ is a compact set then according to Tikhonov, if Equation 1 satisfies (2a), and (2b), there exists a function $\alpha(\tau)$, where τ is a variable parameter, such that

(a) $\alpha(\tau)$ is a continuous nondecreasing function with $\alpha(0) = 0$.

(b) for any $f_1, f_2 \in \Phi$ satisfying the inequality $\rho(Af_1, Af_2) \leq \epsilon$ where $\rho(\psi\phi)$ is the metric or measure of distance between ψ and ϕ and ϵ is a constant, then the following holds

$$\rho(f_1, f_2) \leq \alpha(\epsilon)$$

That is, if a problem is improperly posed in the metric spaces F and U , it becomes properly posed in the usual sense if F is replaced by the subspaces Φ and Φ_A .

The reason for examining the spaces F, U together with Φ, Φ_A is due to the fact that in real problems the errors introduced from experimental measurements into the determination of a set $\{u\}$ usually result in some u being outside Φ_A . The regularization technique formulated by Tikhonov gives the possibility of constructing an approximate solution with a certain guaranteed degree of accuracy even though the exact solution of Equation 1 with approximate data either does not exist or greatly deviates from the "true" solution.

SECTION III

QUADRATIC PROGRAMING

Consider the quadratic programming problem of finding $\{x_i\}$,
 $i = 1, \dots, n$ which maximizes

$$\sum_{i=1}^n b_i x_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n x_i x_j g_{ij} \quad (3)$$

subject to

$$\sum_i c_{ki} x_i \leq d_k ; k = 1, \dots, m \quad (4)$$

and the non-negativity conditions

$$x_i \geq 0 \quad i = 1, \dots, n \quad (5)$$

where g_{ij} are the elements of a symmetric, positive semi-definite matrix,
i. e.,

$$g_{ij} = g_{ji} \quad (6)$$

and

$$\sum_{j=1}^n \sum_{k=1}^n g_{kj} x_j x_k \geq 0 \quad (7)$$

for all x_j . It is always possible to write a quadratic function in the form of Equation 3 such that Equation 6 is satisfied. The restriction Equation 7 ensures that the solution of Equation 3 is convex. There have been many algorithms devised for solving this problem. A few of these are one due to Dantzig (Reference 43), one due to Thiel and Van de Panne (Reference 44), another due to Lemke (Reference 45); two based on extensions of the simplex algorithm encountered in linear programming one by Wolfe (Reference 46) and another by Beale (References 47, 48). In addition, there are excellent review articles and/or books written on the details involved in solving Equations 3, 4, and 5 (References 49-54).

In matrix notation Equations 3 through 5 can be written as maximize,

$$B'X - \frac{1}{2} X'GX \quad (8)$$

subject to

$$CX \leq D \quad (9)$$

and

$$X \geq 0 \quad (10)$$

where G is positive semi-definite, i.e., $X'GX \geq 0$ for all values of X . Here the "prime" indicates the transpose.

The well-known Kuhn-Tucker conditions assert that X is a solution if and only if there exists a vector W such that

$$W \geq 0 \quad (11)$$

$$W'D - W'C X = 0 \quad (12)$$

$$GX + C'W - B \geq 0 \quad (13)$$

and

$$X'GX + X'C'W - X'B = 0 \quad (14)$$

By making the following substitutions

$$V = GX + C'W - B \geq 0 \quad (15)$$

and

$$Y = D - C X \geq 0 \quad (16)$$

the Kuhn-Tucker conditions can then be stated as finding X , W , V and Y , all ≥ 0 , such that

$$\begin{bmatrix} -G & 0 & E & -C' \\ C & E & 0 & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \\ V \\ W \end{bmatrix} = \begin{bmatrix} -B \\ D \end{bmatrix} \quad (17)$$

where E are unit matrices and such that

$$[VW]' \begin{bmatrix} X \\ Y \end{bmatrix} = V'X + W'Y = 0 \quad (18)$$

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In the following sections the method used to incorporate the regularization technique of Tikhonov into the quadratic programming scheme outlined above will be discussed.

SECTION IV

REGULATION OF ILL-POSED INTEGRAL EQUATIONS OF THE FIRST KIND

As an example of the application of Tikhonov's regularization technique, consider a Fredholm integral equation of the first kind,

$$u(\xi) = Q[\xi, f(m)] = \int_{M_0}^{M_1} K(\xi, m)f(m)dm, \xi_0 \leq \xi \leq \xi_1 \quad (19)$$

Assuming that certain $u(\xi)$ functions exist which do not have corresponding $f(m)$ solutions fulfilling conditions (1a), (1b), and (1c), means Equation 19 is an IPP. Then upon application of Tikhonov's ideas (Equation 2) to a special function $\bar{u}(\xi)$ there corresponds a solution:

$$\bar{f}(m) = R[m, u(\xi)] \quad (20)$$

Also let an approximating function $\tilde{u}(\xi)$ for $\bar{u}(\xi)$ be given, such that $||\tilde{u} - \bar{u}|| < \delta$, where δ is known. It is then required to find $\tilde{f}(m)$, an approximation to $\bar{f}(m)$ with an assigned precision $||\tilde{f} - \bar{f}|| \leq \epsilon$ if δ is sufficiently small. Letting $M_0 = 0$; $M_1 = M_{\max}$; $\xi_0 = 0$ and $\xi_1 = 1$; assuming $K(\xi m)$ is continuous and if for $\bar{u}(\xi) = 0$ there exists just one solution $\bar{f}(m) = 0$; then instead of using the conventional functional of calculus of variations

$$N[f(m); \bar{u}(\xi)] = \int_0^1 \left\{ Q[\xi, f(m)] - \bar{u}(\xi) \right\}^2 d\xi \quad (21)$$

Tikhonov suggests application of the functional

$$M_n^\alpha [f(m); \bar{u}(\xi)] = N [f(m); u(\xi)] + \alpha \Omega^{(n)} [f(m)] \quad (22)$$

where $\Omega^{(n)}$ is the regularizing functional

$$\Omega^{(n)}(f) = \int_0^{M_{\max}} \left\{ \sum_{i=0}^{N+1} P_i(m) [f^{(i)}(m)]^2 \right\} dm \quad (23)$$

the $P_i(m)$ are positive continuous functions, $f^{(i)}$ is the i th derivative with respect to m and α is an arbitrary parameter which minimizes the functional M_n^α .

Application of the Eulerean equation and applying boundary conditions results in

$$L_n^\alpha [f] = \alpha \left\{ \sum_{i=0}^{N+1} (-1)^{i+1} \frac{d^i}{dm^i} \left[P_i(m) \frac{d^i f}{dm^i} \right] \right\} - \left\{ \int_0^{M_{\max}} \bar{K}(m, \xi) f(\xi) d\xi - \bar{s}(m) \right\} = 0 \quad (24)$$

with boundary conditions

$$\pi^\ell(m) = \left\{ \sum_{i=\ell+1}^{N+1} (-1)^{i-\ell-1} [P_i(m) f^{(i)}(m)]^{(i-\ell-1)} \right\} \bigg|_{M=0, M_{\max}} = 0 \quad (25)$$

$$(\ell = 1, 2, \dots, N + 1)$$

where

$$\overline{K}(m, \xi) = \int_0^1 K(\xi, m) K(\xi, \xi) d\xi \quad (26)$$

and

$$\overline{s}(m) = \int_0^1 K(\xi, m) \overline{u}(\xi) d\xi \quad (27)$$

This procedure was applied to a kernel of the form

$$K(\xi, s) = \beta s e^{-\beta s \xi} / (1 - e^{-\beta s}) \quad (28)$$

appearing in the theory of equilibrium sedimentation of polydisperse system, by initially assuming $\overline{f}(s) = \text{const.} \times s^2(1-s)^2$, the set $\{\overline{u}\}$ was computed using Equation 19. M_n^α of Equation 22 was then minimized by application of the regularizing technique resulting in the approximate solution $\tilde{f}^\alpha(s)$. Figures 1 and 2 show the results of the computation without regularization and with regularization, respectively (Reference 55).

During the application of this technique to a specific physical problem it was observed that when $\overline{f}(m)$ was multimodal (bimodal or higher) then portions of $\tilde{f}^\alpha(m)$ were negative. From physical considerations of the problem of determining a molecular weight distribution from data obtained from an ultracentrifuge equilibrium sedimentation experiment for which the kernel in Equation 28 is applicable, all $\tilde{f}^\alpha(m)$ should be positive. Using these considerations regularization was incorporated into (LP) linear programming (Reference 56) using Dantzig's Simplex algorithm (Reference 57). The regularized LP technique gave good results up through a trimodal distribution. For higher multimodal distributions

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the computed $\tilde{f}^{\alpha}(m)$ were very erratic and the computational error was large. However, since the functional to be minimized (Equation 22) is quadratic, it seemed only natural to apply quadratic programming.

In the following the incorporation of regularization into the quadratic programming algorithm given by Boot (Reference 54) is discussed.

SECTION V
INCORPORATION OF REGULARIZATION
INTO QUADRATIC PROGRAMING

In all applications involving the kernel given by Equation 28 it has been found that sufficiently satisfactory results were obtained when the $P_i(m)$'s in Equation 23 were equated to constants. Therefore the functional in Equation 22 to be minimized was restricted to become

$$M_n^\alpha [f(m); \bar{u}(\xi)] = N [f(m); \bar{u}(\xi)] + \sum_n \alpha_n \Omega^{(n)} [f] \quad (29)$$

where now

$$\Omega^{(n)} [f] = \int_0^M \max [f^{(n)}(m)]^2 dm \quad (30)$$

$f^{(n)}(m)$ being the n^{th} derivative of $f(m)$ with respect to m , $(f^{(n)}(m) = d^n f(m)/dm^n)$. The n^{th} derivative of $f(m)$ for $n = 1, 2, 3, \dots$ can be approximated by various numerical techniques. In this specific case, assume h is the constant increment associated with the mesh for m . Then $f_j^{(n)}$ can be approximated by

$$f_j^{(n)} = \frac{1}{h^n} \sum_{k=0}^n \binom{n}{k} (-1)^k f_{j-p+k} \quad (31)$$

where $\binom{n}{k}$ are the binomial coefficients; and $p = n$ for n odd; and $p = n-1$ for n even. Then Equation 30 becomes

$$\Omega^{(n)} [f] = \frac{1}{h^{n-1}} \sum_{j=1}^J \sum_{i=1}^J \sum_{k=0}^n \sum_{\ell=0}^n \binom{n}{k} \binom{n}{\ell} (-1)^{\ell+k} f_{j-p+k} f_{i-p+\ell} \quad (32)$$

which in matrix notation will be

$$\Omega^{(n)} [f] = f' \Lambda^{(n)} f \quad (33)$$

where Λ is a matrix whose elements are zero except for diagonal and near off diagonal elements for which if $r = j - p + k$ and $s = i - p + 1$ (as in Equation 32) then

$$\lambda_{r,s}^{(n)} = \sum_{k=0}^n \sum_{\ell=0}^n \binom{n}{k} \binom{n}{\ell} (-1)^{\ell+k} \quad (34)$$

with the boundary conditions $1 \leq r \leq J$ and for $s < 1$, then $s = |s| + 1$ or $s > J$, then $s = 2J - s + 1$.

Next consider Equation 21. Let us express this in matrix notation, where as in Equation 1 the operator (kernel multiplied by appropriate integration constants for numerical evaluation) will be designated by $A = \{a_{ij}\}$; $u = \{u_i\}$ $i = 1, 2, \dots, I$; and $f = \{f_j\}$ $j = 1, 2, \dots, J$. Thus Equation 21 can be expressed as

$$\sum_{i=1}^I \left(\sum_{j=1}^J a_{ij} f_j - u_i \right)^2 = f' A' A f - 2 u' A f + u' u \quad (35)$$

Neglecting the last term in Equation 35 which is a constant, and using the result of Equation 33, the functional M_n^α of Equation 29 expressed in matrix notation is

$$M_n^\alpha = f' A' A f - 2 u' A f + \sum_n \alpha_n f' \Lambda^{(n)} f \quad (36)$$

or upon dividing by 2 to be in correspondence with Equations 3 and 8 and multiplying by (-1), the functional to be maximized will be

$$\bar{M}_n^\alpha = u' A f - \frac{1}{2} f' \left[A' A + \sum_n \alpha_n \Lambda^{(n)} \right] f \quad (37)$$

(Equation 8), subject to $\sum_{j=1}^J t_j f_j \leq \text{const.}$ and all $f_j \geq 0$.

This is now a suitable quadratic program formulation. In the following a particular kernel will be used and a computer simulation experiment where-in analogous experimental data $\{\bar{u} : \bar{u} = A\bar{f}\}$ is generated from an assumed set $\{\bar{f}\}$ and the back solution, determining \tilde{f} from \bar{u} will be discussed. Since in a real experimental situation the original \bar{f} would be unknown, \bar{f} and \tilde{f} are presented only for illustrative purposes. All computations were performed so as to choose that set of α_n 's (usually a single α_n sufficed) which yielded a minimum for $||\bar{u} - u||$ i. e., the error criterion was to choose that $\{\tilde{f}\}_{\alpha_n}$ in correspondence with $\inf \{||\bar{u} - \tilde{u}||\}$.

SECTION VI

APPLICATION AND RESULTS

The first step in proving the utility of Equation 37 was to establish a kernel which represented an IPP in a real physical situation. Such an expression is Equation 28. The computational work was then related to the following integral equation of the first-kind.

$$u(\xi) = \int_0^{m_{\max}} \frac{\beta_m e^{-\beta_m \xi}}{1 - e^{-\beta_m}} f(m) dm \quad (38)$$

where $\beta = \text{const.}$ and $0 \leq \xi \leq 1$. In all cases $\beta = 4 \times 10^{-5}$. For unimodal and trimodal distributions, $\bar{f}(m)$, a 41-point mesh was used for ξ and m ; for a tetramodal distribution a 51-point mesh and for an asymmetrical bimodal and pentamodal a 59-point mesh was used. That is, if N equals the number of intervals in our mesh then $\xi = n_1/N$ where, $n_1 = 1, 2, \dots, N-1$ and $m = n_2 m_{\max}/N$, $n_2 = 1, 2, \dots, N-1$. All integrations were performed using Simpson's quadrature formula for equidistant points. It was felt that in real problems this would be sufficient and it was not the purpose of this research to study how to minimize machine round-off errors.

An initial functional distribution $\bar{f}(m)$, unimodal through pentamodal, was assumed. Then Equation 38 was used to compute a set of values for $\bar{u}(\xi)$. These were then assumed to be our experimental values.

Next, quadratic programming with regularization was applied (Equation 37). For a given α_n , the corresponding set $\{\tilde{f}\}_{\alpha_n}$ which minimized \bar{M}_n^{α} was computed. Then through application of Equation 38 the corresponding set $\{u(\xi)\}_{\alpha_n}$ was evaluated. The α_n which yielded $\inf \{||\bar{u} - \tilde{u}||\}$ was the final α_n used. Further searching for an α_n with more significant digits would have decreased the error analysis criterion but for our purposes two significant figures were considered satisfactory. Finally the initial $\bar{f}(m)$ and the $\tilde{f}^{\alpha}(m)$ were plotted in order to compare the distributions.

These distributions along with the computed data are presented in Figures 2 through 7 and Tables I through V, respectively. To show the need for regularization some figures are presented with the results obtained when no regularization - only quadratic programming was used. In addition it should be noted that the fewer points per mode the less the precision. This is especially noticeable when comparing the unimodal and pentamodal distributions. In the former, 41 points were used per mode whereas in the latter there were only about 11 or 12 points per mode. Due to round-off errors, storage space in a high speed digital computer, and computational time the present computation was limited to using no more than about 11 points per mode for the pentamodal distribution. As a demonstration of this necessity to sample a sufficient number of molecular weights, the following test was performed. Starting with nine molecular weights the initial $\bar{f}(m^*)$ was computed. From these functional values the corresponding set $\bar{u}(\xi^*)$ was inferred on a 41-point mesh. This number of values was used to compute the corresponding set $\tilde{f}^\alpha(m^*)$, in the same fashion as $\bar{f}(m^*)$. Finally, the set $\tilde{f}^\alpha(m^*)$ was used to compute an analogous set $\tilde{u}(\xi^*)$. Figure 8 shows a comparison of $\bar{u}(\xi)$ computed from the $\bar{f}(m)$ with 41 molecular weight (Figure 3) with $\bar{u}(\xi^*)$ and $\tilde{u}(\xi^*)$ computed using a nine-point molecular weight mesh.

SECTION VII

CONCLUSIONS

The need for knowing the molecular weight distribution of synthetic polymers first led the authors to the ill-posed inverse problem associated with Equation 38. Scientists have investigated the feasibility of this determination for the past 30 to 40 years. All types of well founded mathematical theories were applied, but each would, in general, only be applicable for specific types of distributions. It was only recently realized that, instead of apologizing for the kernel of Equation 38 being ill-conditioned, the entire problem was mathematically ill-posed in the Hadamard sense. It should be challenging to derive another expression for determining a molecular weight distribution from equilibrium sedimentation data which might be a well-posed problem. Meantime, (since time and economics prevented such a diversion) application of Tikhonov's technique of regularization has enabled reliable results to be obtained. Good results were obtained for unimodal through tetramodal distributions. Poor results were obtained for a pentamodal distribution. The results indicate that even if the experimental data $u(\xi)$ are precise, a "poor fit" MWD will be obtained if the sampling size of molecular weights is too small. It can be estimated that a lower limit on the number of molecular weights per mode or per peak has to be about 20 in order to obtain a good "fit". Ten molecular weights per peak gave poor results. To assure such a good "fit" a bimodal distribution would require a 40-point mesh minimum. Unfortunately, because of the computer storage limitations, as well as an extensive computation time, the mesh could not exceed 61 points. This number was adequate to compute a trimodal, barely adequate to compute a tetramodal distribution, and entirely inadequate to compute a pentamodal distribution. Considering these limitations, the computation of higher multimodal distributions were not attempted.

In addition, a larger molecular weight mesh would also require a corresponding larger number of discernible $u(\xi)$. For the ultracentrifugal techniques this would require the use of longer column lengths for solutions investigated.

APPENDIX

QUADRATIC PROGRAM ALGORITHM

Computer programs were written to solve the following problems. Find the values of x_1, x_2, \dots, x_n that maximize

$$(a_1 \ a_2 \ \dots \ a_n) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} - \frac{1}{2} (x_1 \ x_2 \ \dots \ x_n) \begin{bmatrix} b_{11} & b_{12} & b_{1n} \\ b_{21} & b_{22} & b_{2n} \\ \vdots & \vdots & \vdots \\ b_{n1} & b_{n2} & b_{nn} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

subject to

$$\begin{bmatrix} c_{11} & c_{12} & c_{1n} \\ c_{21} & c_{22} & c_{2n} \\ \vdots & \vdots & \vdots \\ c_{k1} & c_{k2} & c_{kn} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \leq \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_k \end{pmatrix}$$

$$x_i \geq 0 \quad i = 1, 2, \dots, n$$

where

$$\begin{bmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ b_{21} & b_{22} & \dots & b_{2n} \\ \dots & \dots & \dots & \dots \\ b_{n1} & b_{n2} & \dots & b_{nn} \end{bmatrix} \text{ is positive semi-definite}$$

In matrix form we have:

Find the value of x' that maximizes

$$A'x - 1/2 x' Bx$$

subject to

$$\begin{aligned} CX &\leq D \\ X &\geq 0 \end{aligned}$$

where B is positive semi-definite, i. e., $X'BX \geq 0$ for all values of X. This problem can be reformulated by introducing k non-negative slack variables $(y_1 y_2 \dots y_k)' = Y$ (Reference 53), and stating the problem as: Find the values of X, Y that maximize

$$[A \ 0] \begin{bmatrix} X \\ Y \end{bmatrix} - \frac{1}{2} [X \ Y] \begin{bmatrix} B & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}$$

subject to

$$\begin{aligned} [C \ I] \begin{bmatrix} X \\ Y \end{bmatrix} &= D \\ X &\geq 0 \\ Y &\geq 0 \end{aligned}$$

Using the Kuhn-Tucker conditions, it can be shown that $[X \ Y]'$ where prime denotes transpose, is the solution to this problem if and only if

1. $[X \ Y]' \geq 0$
2. There exists a vector $[V \ W]$ of non-negative elements such that

$$[V \ W]' \begin{bmatrix} X \\ Y \end{bmatrix} = V'X + W'Y = 0$$

3. The vectors $[X \ Y]'$ and $[V \ W]'$ satisfy the system of linear equations

$$\begin{bmatrix} -B & 0 & I & -C' \\ C & I & 0 & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \\ V \\ W \end{bmatrix} = \begin{bmatrix} -A \\ D \end{bmatrix}$$

Dantzig's algorithm as presented by Boot (Reference 53) is used. The procedure begins with a basic feasible standard form solution $(X \ Y \ V \ W)' = (0 \ D \ -A \ 0)'$ of the system of linear equations above. The system of linear equations has $m + k$ equations and $2(m + k)$ unknowns.

A basic solution is a solution determined by setting $m + k$ of the variables equal to zero and solving the remaining variables. A basic feasible solution is a basic solution that has only non-negative values for $[X \ Y]$. Standard and nonstandard basic feasible solutions are defined as follows. Let $Z' = [X \ Y]'$ and $U' = [V \ W]'$. If a basic feasible solution is such that no pair of corresponding Z and U variables consist of two nonzero elements, the solution is in standard form, otherwise the basic feasible solution is in nonstandard form.

In a basic feasible solution of the system of linear equations, the variables that are set equal to zero are called nonbasis variables, the remaining are called basis variables and comprise the basis. The algorithm consists of adding a variable to the basis and deleting a variable from the basis. This is better explained by writing the system of linear equations as a linear combination of vectors equal to a vector.

Let P_m equal the m^{th} column of the matrix

$$\begin{bmatrix} -B & O & I & -C' \\ C & I & O & O \end{bmatrix}$$

and let $P'_0 = [-A \ D]$. Then the system of linear equations can be written

$$Z_1 P_1 + Z_2 P_2 + \dots + Z_{n+k} P_{n+k} + U_1 P_{n+k+1} + U_2 P_{n+k+2} + \dots + U_{n+k} P_{2n+2k} = P_0$$

Let P_m , $m = 1, 2, \dots, n + k$ be the values of the basis variables and let j_m = the subscript of the associated P vector for the m th basis variable $m = 1, 2, \dots, n + k$

The rules for adding a variable to the basis are:

1. If the basic feasible solution is in standard form, that particular non-basic Z -variable should enter the basis whose corresponding U_h has (in absolute value) the largest negative P_h .
2. If the basis feasible solution is nonstandard and (Z_k, U_k) is the nonbasic pair, then U_k should enter the basis.

Let the P vector corresponding to the variable that is to enter the basis be represented by $(T_1 \ T_2 \ \dots \ T_{n+k})'$. The rules for deleting a variable from the basis are:

1. If the basic feasible solution is standard, let Z_h be the variable that is to enter the basis. Find the value of m that corresponds to the smallest positive ratio P_m/T_m while only considering those m 's such that $j_m \in \{1, 2, \dots, n+k, n+k+h\}$.
2. If the basic feasible solution is nonstandard, let (Z_h, U_h) correspond to the pair that are both basic. Find the value of m that corresponds to the smallest positive ratio P_m/T_m while only considering those m 's such that $j_m \in \{1, 2, \dots, n+k, n+k+h\}$.

The algorithmic recycling is terminated when all of the basic variables are nonnegative, i. e., when $P_m \geq 0$; $m = 1, 2, \dots, n+k$.

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TABLE I
COMPUTATIONAL RESULTS FOR THE UNIMODAL DISTRIBUTION
FROM A 41-POINT MESH

No.	m	$\bar{f}(m) \times 10^6$	$\hat{f}^a(m) \times 10^6$	$\bar{u}(\xi)$	$\hat{u}(\xi)$
1	3,571	0.108	0.200	3.2052	3.2061
3	10,714	0.880	0.791	2.7151	2.7159
5	17,857	2.200	2.170	2.3069	2.3075
7	25,000	3.858	3.931	1.9660	1.9664
9	32,143	5.670	5.737	1.6806	1.6809
11	39,286	7.474	7.460	1.4410	1.4413
13	46,429	9.135	9.061	1.2393	1.2396
15	53,571	10.542	10.477	1.0692	1.0694
17	60,714	11.609	11.623	0.9252	0.9254
19	67,857	12.274	12.356	0.8031	0.8033
21	75,000	12.500	12.578	0.6992	0.6993
23	82,143	12.274	12.276	0.6106	0.6107
25	89,286	11.609	11.523	0.5348	0.5349
27	96,429	10.542	10.438	0.4698	0.4699
29	103,570	9.135	9.095	0.4139	0.4140
31	110,710	7.474	7.554	0.3657	0.3658
33	117,860	5.670	5.813	0.3240	0.3241
35	125,000	3.858	3.912	0.2879	0.2880
37	132,140	2.200	2.076	0.2565	0.2566
39	139,290	0.880	0.761	0.2291	0.2292
41	146,430	0.108	0.270	0.2052	0.2053

$$\alpha_2 = 5.8 \times 10^{-6}$$

$$\|\bar{u} - \hat{u}\| = 3.35 \times 10^{-4}$$

$$\xi = \text{Number}/43$$

TABLE II
COMPUTATIONAL RESULTS FOR THE ASYMMETRICAL BIMODAL
DISTRIBUTION FROM A 59-POINT MESH

No.	m	$\bar{f}(m) \times 10^6$	$\tilde{f}^a(m) \times 10^6$	$\bar{u}(\xi)$	$\tilde{u}(\xi)$
1	2,500	0.173	0.110	2.8642	2.8644
3	7,500	1.388	1.565	2.5625	2.5727
5	12,500	3.401	3.639	2.3163	2.3164
7	17,500	5.834	5.484	2.0906	2.0908
9	22,500	8.259	7.587	1.8915	1.8916
11	27,500	10.706	10.483	1.7154	1.7156
13	32,500	12.656	13.181	1.5594	1.5595
15	37,500	14.047	15.050	1.4208	1.4209
17	42,500	14.769	15.621	1.2975	1.2976
19	47,500	14.769	14.808	1.1875	1.1876
21	52,500	14.047	13.408	1.0891	1.0892
23	57,500	12.656	11.481	1.0010	1.0010
25	62,500	10.706	9.538	0.9218	0.9216
27	67,500	8.359	7.974	0.8506	0.8506
29	72,500	5.834	6.434	0.7863	0.7863
31	77,500	3.520	4.863	0.7282	0.7282
33	82,500	2.316	3.853	0.6756	0.6756
35	87,500	2.385	2.926	0.6278	0.6278
37	92,500	3.670	2.530	0.5844	0.5844
39	97,500	5.057	3.567	0.5448	0.5448
41	102,500	6.184	5.749	0.5086	0.5086
43	107,500	6.914	7.600	0.4755	0.4755
45	112,500	7.167	7.632	0.4452	0.4452
47	117,500	6.914	6.817	0.4173	0.4173
49	122,500	6.184	6.124	0.3917	0.3917
51	127,500	5.057	4.902	0.3681	0.3681
53	132,500	3.670	3.765	0.3463	0.3463
55	137,500	2.212	2.483	0.3261	0.3261
57	142,500	0.929	0.964	0.3075	0.3074
59	147,500	0.119	0.000	0.2902	0.2901

$$\alpha_2 = 7.9 \times 10^{-7} \quad \| \bar{u} - \tilde{u} \| = 8.73 \times 10^{-5}$$

$$\alpha_3 = 5.6 \times 10^{-10} \quad \xi = \text{Number}/61$$

TABLE III
COMPUTATIONAL RESULTS FOR THE TRIMODAL DISTRIBUTION
FROM A 41-POINT MESH

No	m	$\bar{f}(m) \times 10^6$	$\tilde{f}(m) \times 10^6$	$\bar{u}(\xi)$	$\tilde{u}(\xi)$
1	3,571	0.585	0.839	3.2501	3.2524
3	10,714	3.964	3.584	3.7147	2.7165
5	17,857	7.918	8.440	2.2798	2.2812
7	25,000	10.452	10.613	1.9252	1.9264
9	32,143	10.553	9.861	1.6351	1.6360
11	39,286	8.182	7.536	1.3967	1.3975
13	46,429	4.283	4.940	1.2001	1.2008
15	53,571	2.939	4.344	1.0372	1.0379
17	60,714	6.171	6.339	0.9017	0.9022
19	67,857	0.546	8.499	0.7884	0.7889
21	75,000	10.834	9.239	0.6932	0.6937
23	82,143	9.546	8.936	0.6129	0.6133
25	89,286	6.171	7.550	0.5447	0.5452
27	96,429	2.939	5.541	0.4867	0.4871
29	103,570	4.283	4.221	0.4369	0.4373
31	110,710	8.182	5.608	0.3941	0.3945
33	117,860	10.553	0.552	0.3570	0.3574
35	125,000	10.452	11.789	0.3248	0.3252
37	132,140	7.918	8.845	0.2966	0.2970
39	139,290	3.964	3.223	0.2719	0.2723
41	146,430	0.585	0.787	0.2501	0.2504

$$\alpha_2 = 1.0 \times 10^{-6} \quad \| \bar{u} - \tilde{u} \| = 8.5029 \times 10^{-4}$$

$$\alpha_3 = 3.2 \times 10^{-9} \quad \xi = \text{Number}/43$$

$$\alpha_4 = 1.0 \times 10^{-6}$$

TABLE IV
COMPUTATIONAL RESULTS FOR THE TETRAMODAL DISTRIBUTION
FROM A 53-POINT MESH

No.	m	$\bar{f}(m) \times 10^6$	$\tilde{f}(m) \times 10^6$	$\bar{u}(\xi)$	$\tilde{u}(\xi)$
1	2,778	0.592	0.000	3.2556	3.2556
3	8,333	3.991	3.374	2.8297	2.8297
5	13,889	7.910	11.405	2.4678	2.4678
7	19,444	10.329	12.895	2.1595	2.1595
9	25,000	10.251	6.929	1.8964	1.8963
11	30,556	7.706	0.000	1.6712	1.6711
13	36,111	3.807	2.223	1.4780	1.4780
15	41,667	3.064	8.468	1.3120	1.3119
17	47,222	6.616	13.278	1.1688	1.1688
19	52,778	9.731	13.488	1.0450	1.0450
21	58,333	10.583	9.582	0.9378	0.9378
23	63,889	8.841	3.356	0.8446	0.8445
25	69,444	5.199	0.000	0.7633	0.7633
27	75,000	2.754	0.593	0.6923	0.6923
29	80,556	5.199	3.511	0.6300	0.6300
31	86,111	8.841	11.522	0.5752	0.5753
33	91,667	10.583	16.024	0.5269	0.5270
35	97,222	9.731	14.384	0.4842	0.4842
37	102,780	6.616	7.620	0.4463	0.4463
39	108,330	3.064	1.743	0.4126	0.4126
41	113,890	3.807	0.000	0.3824	0.3825
43	119,440	7.706	1.256	0.3555	0.3555
45	125,000	10.251	9.745	0.3312	0.3313
47	130,560	10.329	16.270	0.3094	0.3095
49	136,110	7.910	10.028	0.2897	0.2898
51	141,670	3.991	2.310	0.2718	0.2719
53	147,220	0.592	0.000	2.556	0.2557

$$\alpha_2 = 2.1 \times 10^{-7} \quad \|\bar{u} - \tilde{u}\| = 4.0120 \times 10^{-5}$$

$$\alpha_3 = 7.0 \times 10^{-10} \quad \xi = \text{Number}/55$$

TABLE V
COMPUTATIONAL RESULTS FOR THE PENTAMODAL DISTRIBUTION
FROM A 59-POINT MESH

No.	m	$\bar{f}(m) \times 10^6$	$\tilde{f}^a(m) \times 10^6$	$\bar{u}(\xi)$	$\tilde{u}(\xi)$
1	3,000	0.593	2.609	3.8132	3.8089
3	9,000	3.853	2.747	3.2709	3.2683
5	15,000	7.245	8.257	2.8166	2.8153
7	21,000	8.742	12.430	2.4351	2.4347
9	27,000	7.606	9.559	2.1138	2.1141
11	33,000	4.391	5.370	1.8425	1.8433
13	39,000	2.281	2.880	1.6128	1.6139
15	45,000	4.922	3.231	1.4177	1.4190
17	51,000	7.923	7.604	1.2516	1.2529
19	57,000	8.687	4.621	1.1096	1.1110
21	63,000	6.843	4.082	0.9880	0.9892
23	69,000	3.329	6.802	0.8834	0.8845
25	75,000	2.592	10.928	0.7931	0.7941
27	81,000	5.935	5.983	0.7150	0.7159
29	87,000	8.410	0.000	0.6471	0.6478
31	93,000	8.410	4.985	0.5879	0.5885
33	99,000	5.935	11.253	0.5362	0.5366
35	105,000	2.592	20.421	0.4907	0.4910
37	111,000	3.329	1.102	0.4507	0.4509
39	117,000	6.843	0.000	0.4153	0.4154
41	123,000	8.687	0.000	0.3839	0.3838
43	129,000	7.923	0.000	0.3560	0.3558
45	135,000	4.922	14.118	0.3310	0.3308
47	141,000	2.281	4.616	0.3087	0.3083
49	147,000	4.391	1.905	0.2886	0.2881
51	153,000	7.606	14.409	0.2704	0.2699
53	159,000	8.742	7.154	0.2540	0.2534
55	165,000	7.245	0.000	0.2391	0.2385
57	171,000	3.853	0.000	0.2256	0.2249
59	177,000	0.593	7.073	0.2132	0.2125

$$\alpha_2 = 4.0 \times 10^{-10} \quad \| \bar{u} - \tilde{u} \| = 1.1093 \times 10^{-3}$$

$$\alpha_3 = 1.5 \times 10^{-8} \quad \xi = \text{Number}/61$$

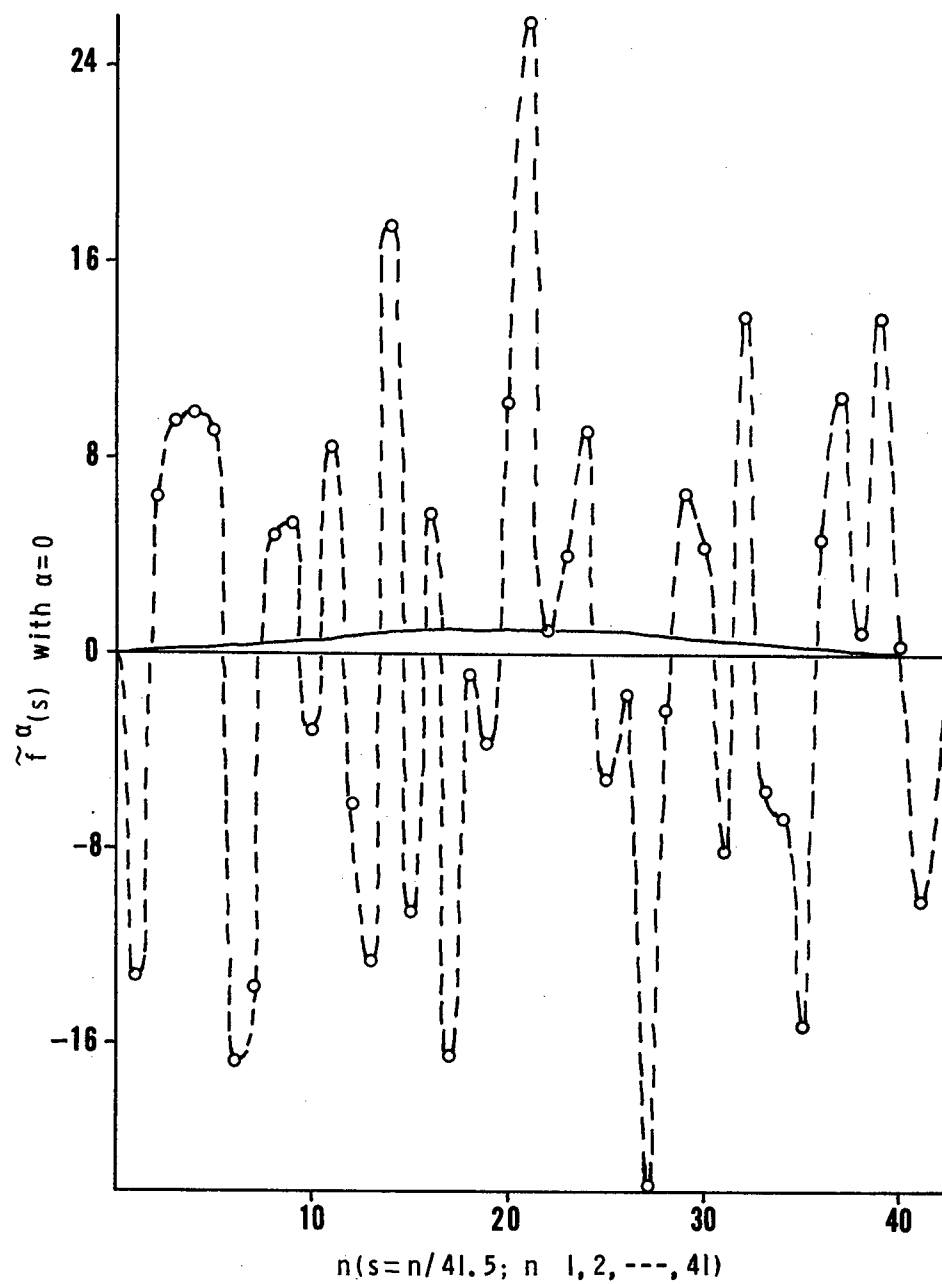


Figure 1. Unimodal Distribution by Variational Calculus without Regularization

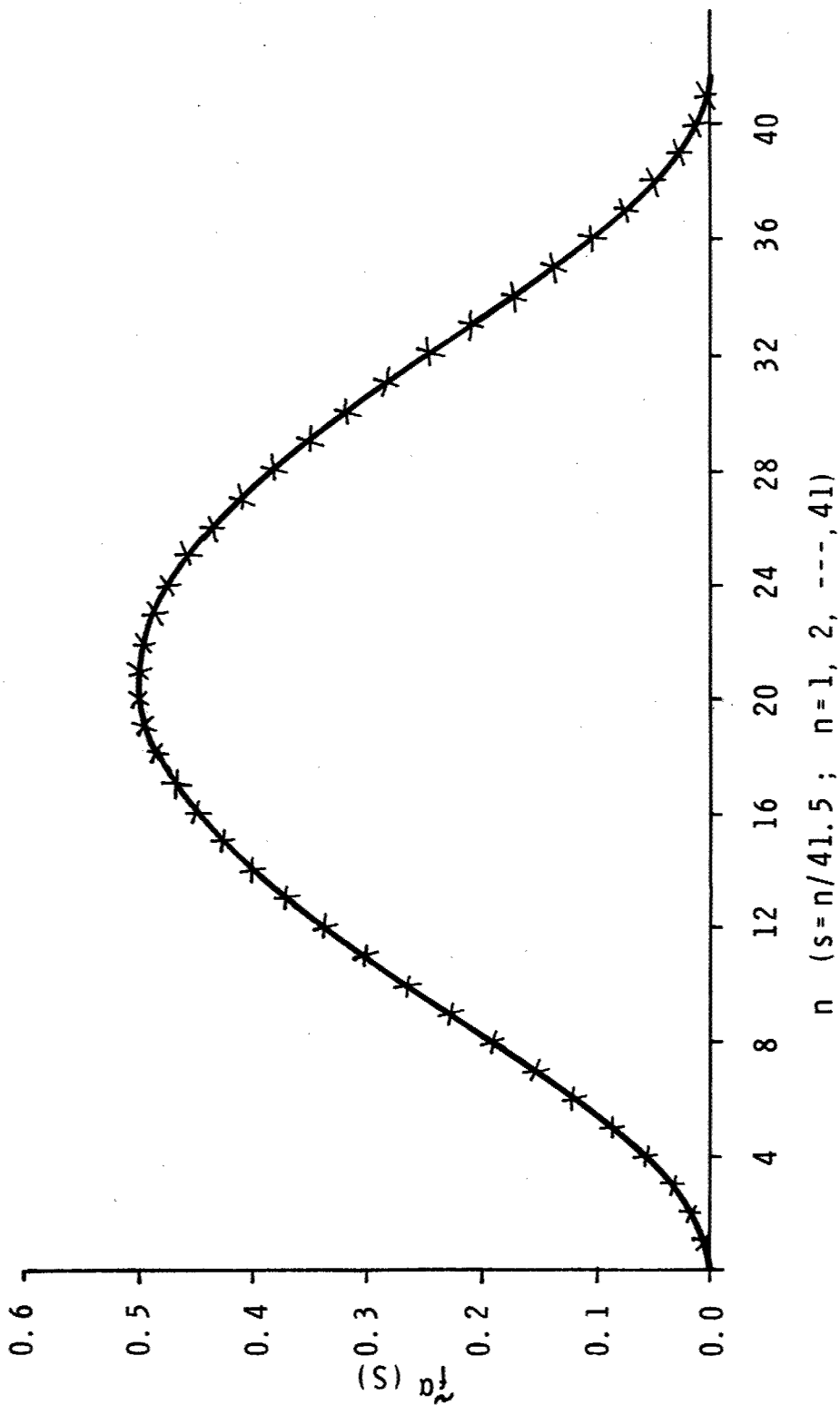


Figure 2. Unimodal Distribution by Variational Calculus with Regularization

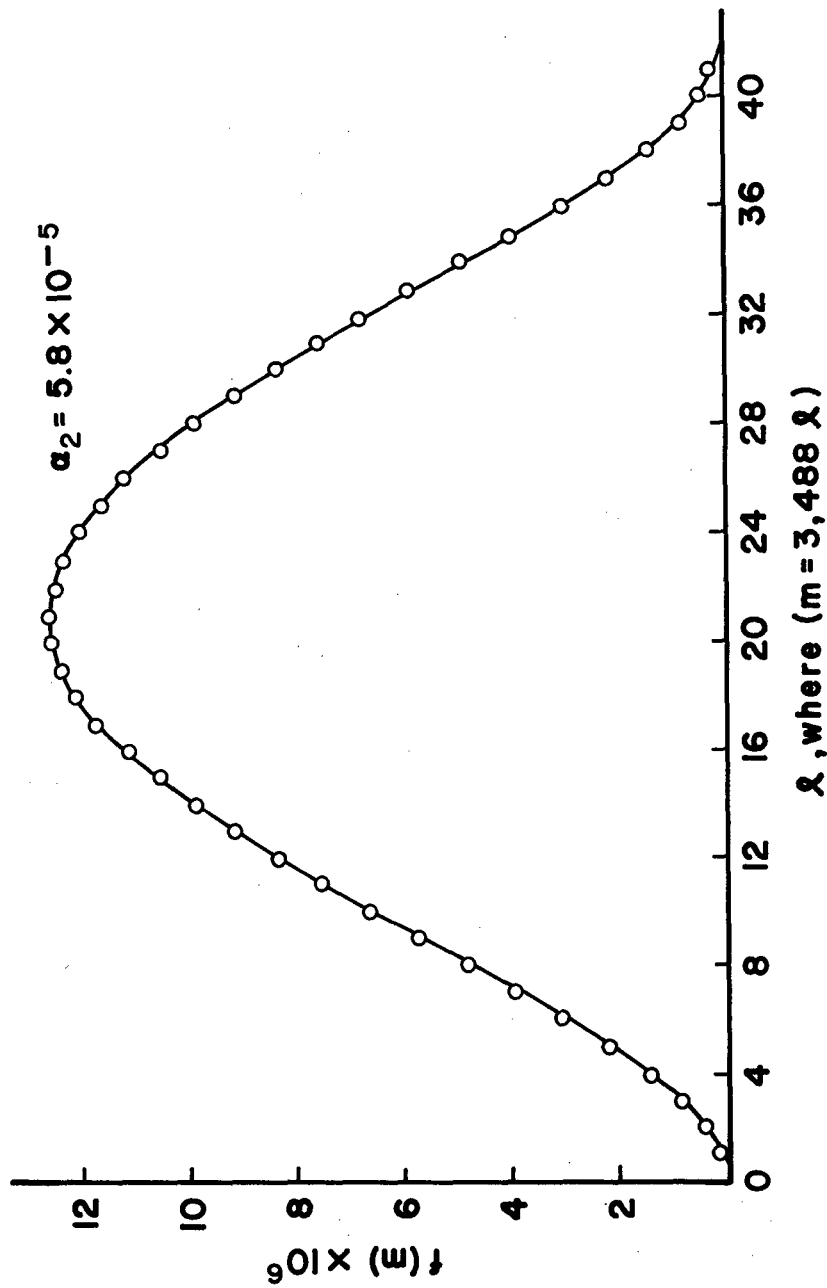


Figure 3. Unimodal Distribution by Regularization and Quadratic Programming. Solid Curve is the Original Distribution, Circles the Resulting Distribution Based on a 41-Point

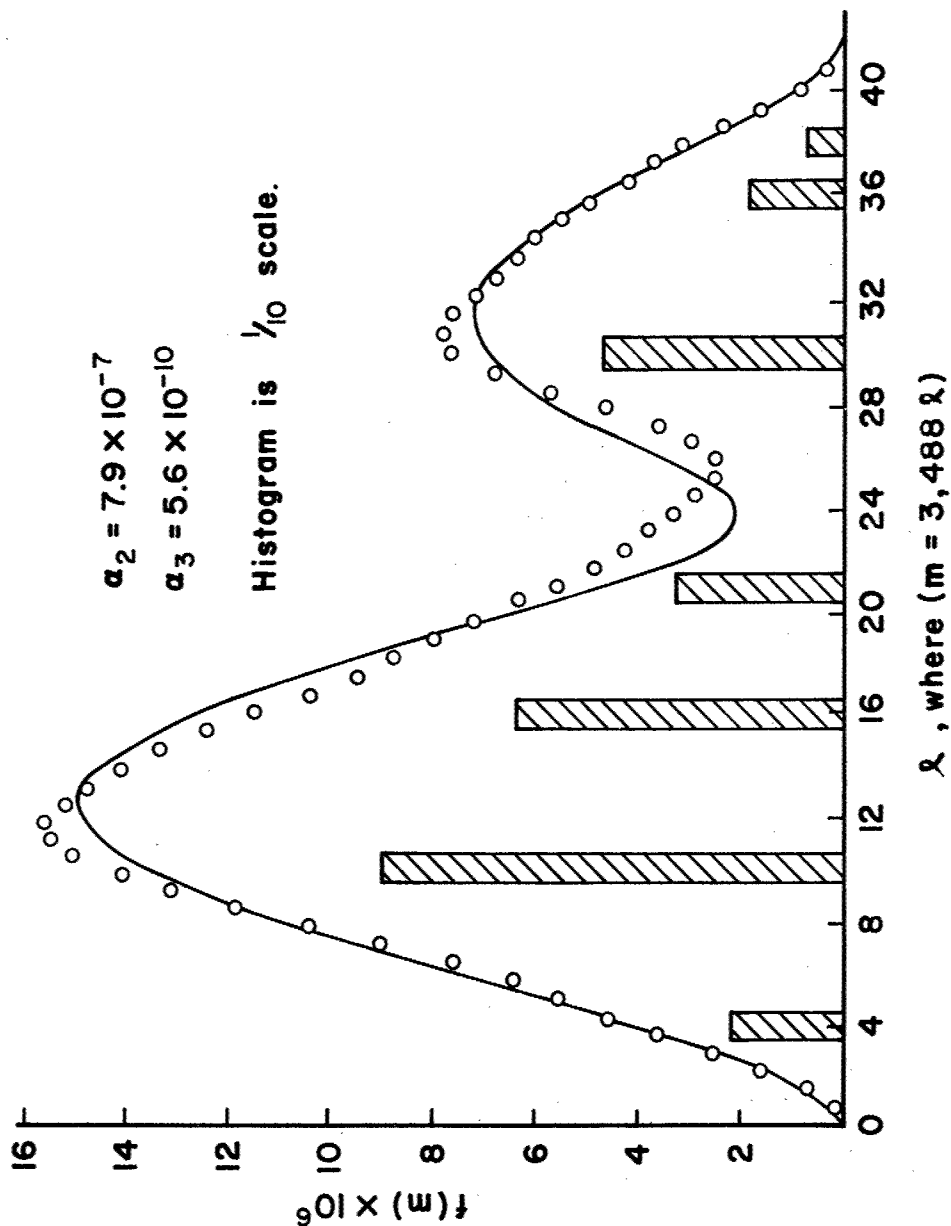


Figure 4. Asymmetrical Bimodal Distribution, Solid Line Represents the Original Distribution, Circles the Distribution by Using a 41-Point Mesh and Regularization with Quadratic Programming. The Histogram to 1/10 Scale Represent Results Using Quadratic Programming without Regularization.

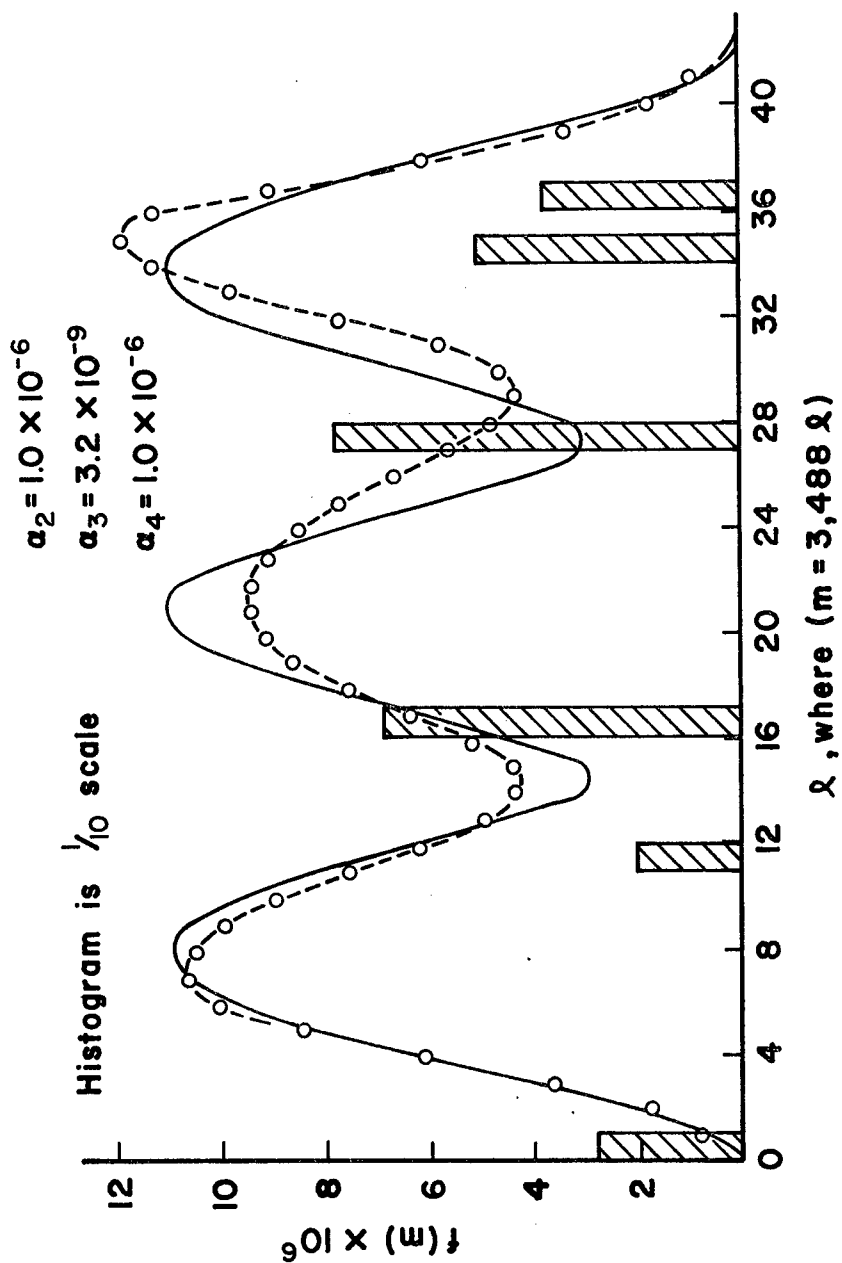


Figure 5. Symmetrical Trimodal Distribution, Solid Line the Original Distribution, the Circles Quadratic Programming and Regularization, the Histogram to $1/10$ Scale Using Only Quadratic Programming

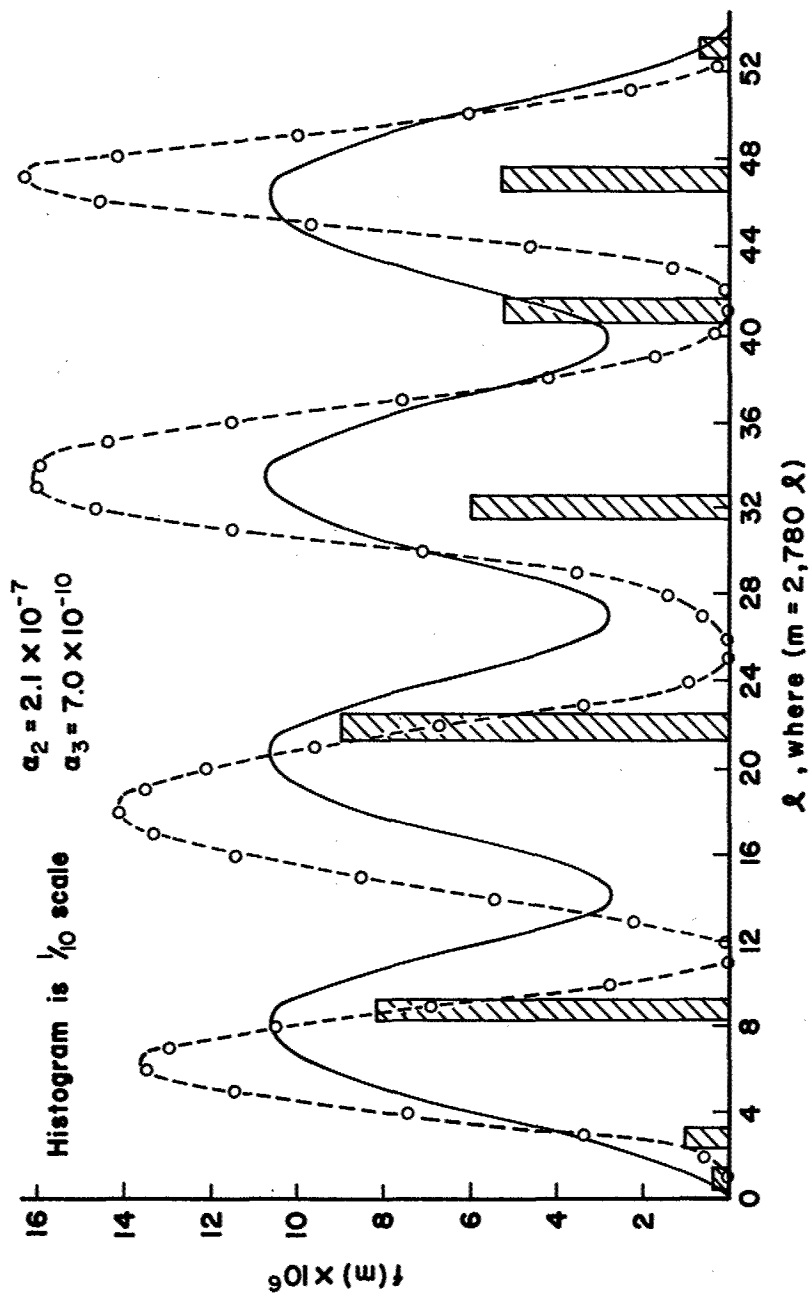


Figure 6. Symmetrical Tetramodal Distribution, Solid Line the Original Distribution, the Circles Quadratic Programming with Regularization, the Histogram to $1/10$ Scale Only Quadratic Programming

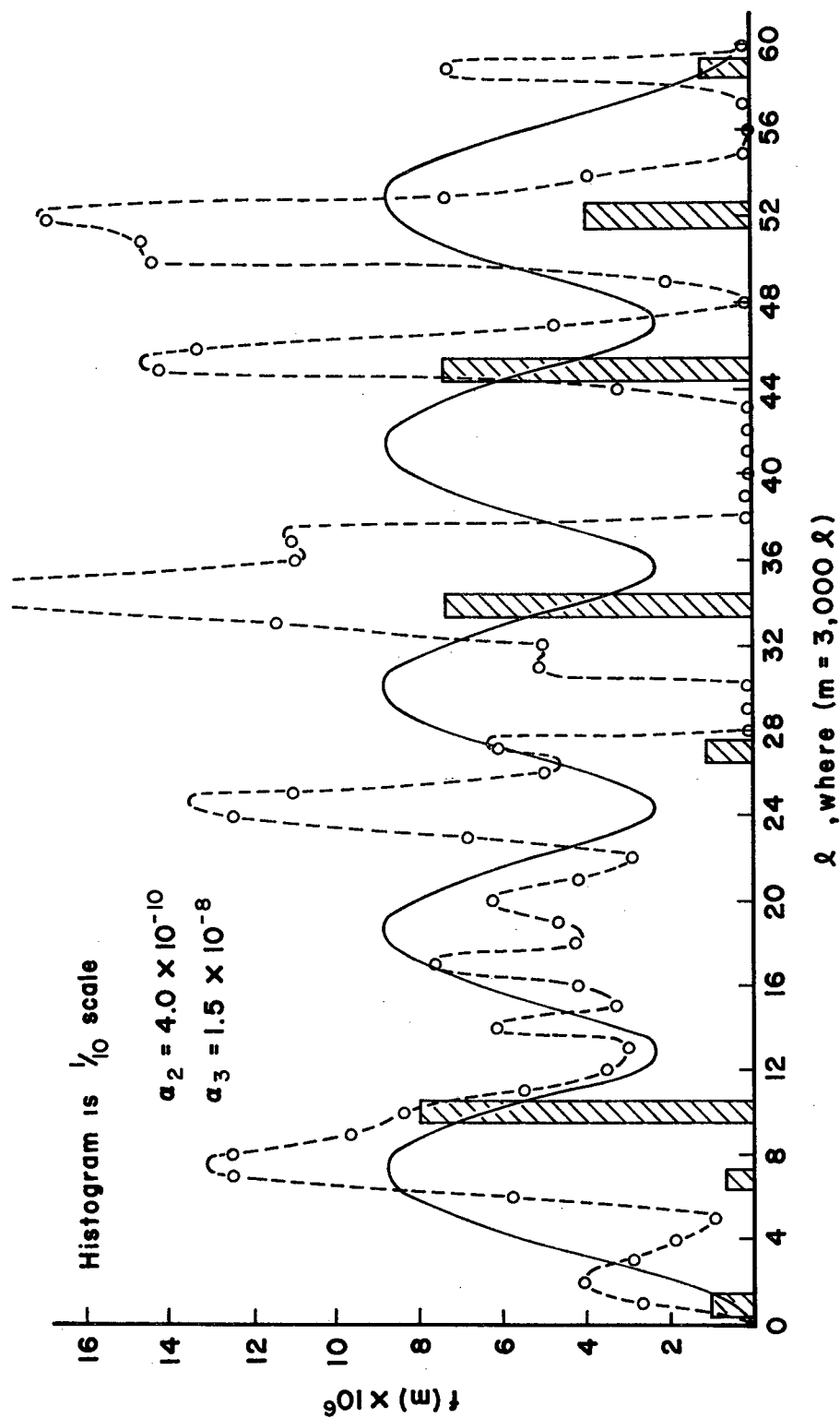


Figure 7. Symmetrical Pentamodal Distribution, Solid Line the Original Distribution, the Circles Quadratic Programming with Regularization, the Histogram to 1/10 Scale Only Quadratic Programming

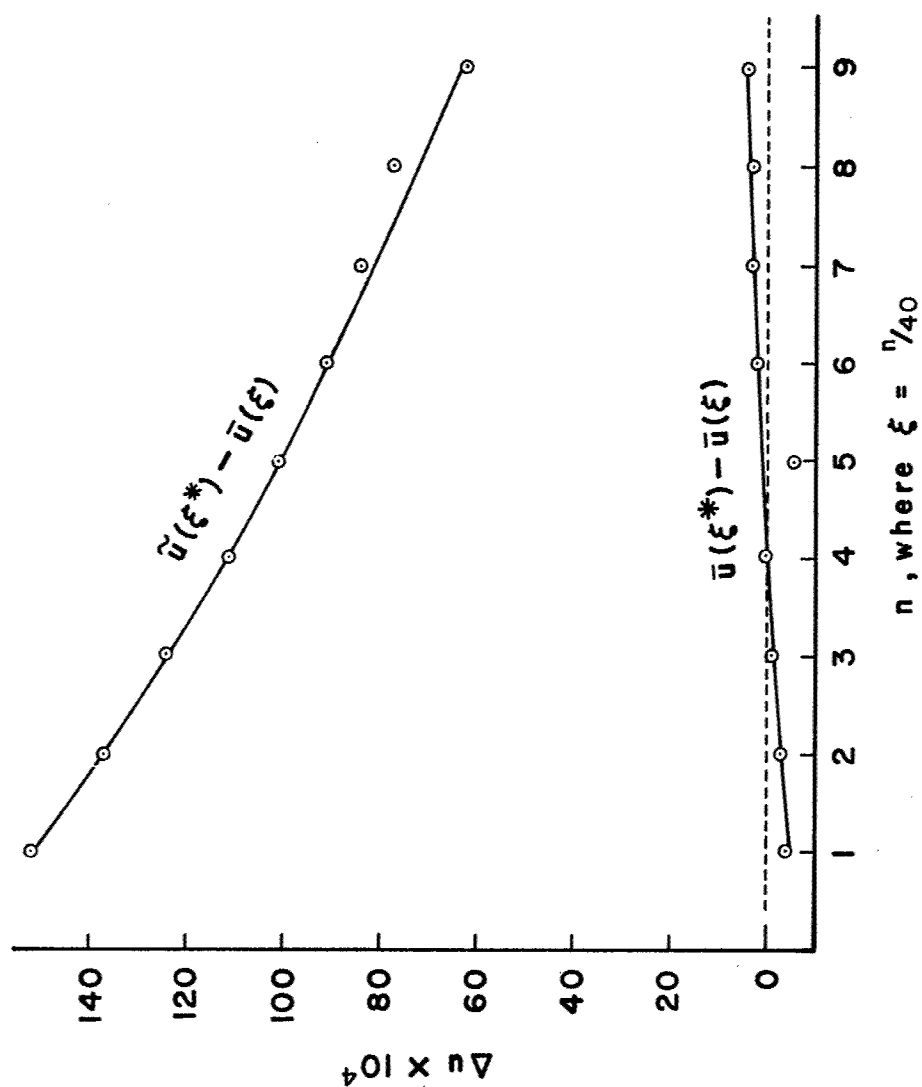


Figure 8. Deviations of the Computed Curve $\bar{u}(\xi^*)$ and $\bar{u}(\xi)$ from the "true" $\bar{u}(\xi)$ as a function of ξ

PROGRAM LISTING

```

C *****
C
C PROGRAM REQUAD
C
C PURPOSE
C   PROGRAM READS ALPHA(NLAST) AS DATA FROM NFIRST
C   THROUGH NCODE. THEN PROGRAM CONTINUES FROM
C   NCODE+1 THROUGH NUPP SEARCHING FOR MINIMUM FOR
C   EACH DERATIVE RETAINING PREVIOUS VALUES. IF
C   NCODE = 0 , SEARCH BEGINS WITH NFIRST.
C   IF NFLAG.GT.0 PROGRAM READS ONE VALUE OF ALPHA AND
C   COMPUTES FOR ONLY THIS ONE VALUE
C
C USAGE
C   PROGRAM REQUAD(TAPE5,OUTPUT,TAPE6=OUTPUT)
C
C   PROGRAM REQUAD(TAPE5,OUTPUT,TAPE6=OUTPUT)
C   COMMON/ZYT/U,XK,S,X,Z,BK,B,ZP,A,ALPHA,R,XX,UP,DLX,DLS,
C   *IMAX,NMAX,NF
C   1RST,NLAST,FACT0,TCOST,TPIV
C   DIMENSIONS FOR COMMON
C   DIMENSION U(60),XK(60,60),S(60),X(60),Z(60),BK(60,60),
C   *B(60),ZP(60)
C   1,A(60,60),ALPHA(10),R(60),XX(60),UP(60)
C   DIMENSION IBASIS(60),RESULT(60)
C
C   READ(5,200)
C   WRITE(6,1000)
C   WRITE(6,200)
C   WRITE(6,1001)
C   NMAX AND IMAX MUST BE ODD INTEGERS
C   READ(5,201) NNMAX,IIMAX,W1,W2
C   NMAX = NNMAX - 2
C   LMAX = NMAX + 1
C   IMAX = IIMAX
C   DLS = FLOAT(NNMAX-1)/(W2-W1)
C   DLX = FLOAT(IIMAX-1)
C   DO 1 I = 1,IMAX
C   X(I) = FLOAT(I-1)/DLX
C 1 CONTINUE
C   COF = 0.
C   DO 2 I = 1,NMAX
C   S(I) = W1 + FLOAT(I)/DLS
C   F1 = 0.
C   IF(S(I).GT.W2.OR.S(I).LT.W1) GO TO 53
C   A1 = (S(I) - W1)**2
C   A2 = (S(I) - W2)**2

```

```

      F1 = A1*A2
53  Z(I) = F1
      KNUM = I/2
      JNUM = (I+1)/2
      IF(JNUM.NE.KNUM) GO TO 51
      SIG = 2.
      GO TO 52
51  SIG = 4.
52  COF = COF + SIG*Z(I)/(3.*DLS)
      2 CONTINUE
      DO 5 I = 1,NMAX
5  Z(I) = Z(I)/COF
C      XSIG = LAMBDA IN THE THEORY, SEE FUJITA'S EQUATION
      READ(5,103) XSIG
      DO 4 I = 1,IMAX
      COEF = 0.
      DO 3 J = 1,NMAX
      A1 = XSIG*S(J)
      A2 = A1
      A3 = EXP(-A1*X(I))
      A4 = EXP(-A1)
      A5 = 1. - A4
      A6 = A2*A3/A5
      XK(I,J) = A5
      KNUM = J/2
      JNUM = (J+1)/2
      IF(JNUM.NE.KNUM) GO TO 42
      SIG = 2.
      GO TO 43
42  SIG = 4.
43  COEF = COEF + SIG*XK(I,J)*Z(J)/(3.*DLS)
      3 CONTINUE
C      CALCULATION OF U(ZI) BY SIMPSON'S FORMULA
4  U(I) = COEF
      CALL REG2
81  CONTINUE
      READ(5,101) NCODE,NFIRST,NUPP,NFLAG,FACT0,TCOST,TPIV
      DO 30 NLAST = NFIRST,NUPP
      IF(NLAST.LE.NCODE) GO TO 31
      IF(NFLAG.GT.0) GO TO 40
      READ(5,100) LPHA1,LPHA2
      LXP = IABS(LPHA2 - LPHA1) + 1
      NUM = 0
      DO 20 II = 1,LXP
      IXP = LPHA1 + II - 1
      DO 21 KL = 1,9
      ALPHA(NLAST) = FLOAT(KL)*10.**IXP
C      OBTAIN MODIFIED MATRIX
      CALL REG3

```

```

C      OBTAIN INVERSE SOLUTION
      CALL QUAD1(RESULT,IBASIS)
      DO 33 I = 1,LMAX
33     ZP(I) = 0.
      DO 32 I = 1,LMAX
      J = IBASIS(I)
      IF(J.GT.LMAX) GO TO 32
      ZP(J) = RESULT(I)
32     CONTINUE
C      EVALUATE ERROR
      CALL REG4(UAVG)
      WRITE(6,4000) ALPHA(NLAST),UAVG
4000  FORMAT(1H ,1P2E12.5)
      IF(KL.EQ.1.AND.II.EQ.1) GO TO 22
      IF(UAVG.GE.AVG1) GO TO 28
      AVG1 = UAVG
C      STORE MINIMUM ERROR AND CORRESPONDING ALPHA
      XM = ALPHA(NLAST)
      NX = IXP
      NUM = 0
      GO TO 21
22     AVG1 = UAVG
C      STORE FIRST ALPHA USED AND ASSOCIATED ERROR
      XM = ALPHA(NLAST)
      NX = IXP
      GO TO 21
28     CONTINUE
21     CONTINUE
20     CONTINUE
23     CONTINUE
      IF(XM.EQ.10.**NX) GO TO 60
      XMM = XM - 10.**NX
      GO TO 62
60     XMM = 9.*10.**(NX-1)
62     CONTINUE
      DO 25 I = 1,20
      ALPHA(NLAST) = XMM + FLOAT(I-1)*10.**(NX-1)
      CALL REG3
      CALL QUAD1(RESULT,IBASIS)
      DO 55 K = 1,LMAX
55     ZP(K) = 0.
      DO 56 K = 1,LMAX
      J = IBASIS(K)
      IF(J.GT.LMAX) GO TO 55
      ZP(J) = RESULT(K)
56     CONTINUE
      CALL REG4(UAVG)
      IF(I.EQ.1) GO TO 26
      IF(UAVG.GE.AVG1) GO TO 25

```

```

      AVG1 = UAVG
      XM = ALPHA(NLAST)
      GO TO 25
26  AVG1 = UAVG
      XM = ALPHA(NLAST)
25  CONTINUE
27  ALPHA(NLAST) = XM
      GO TO 61
40  READ(5,102) ALPHA(NLAST)
C      IF COMPUTATION PROCEEDS FOR ONLY ONE ALPHA BEGIN
C      HERE
61  CONTINUE
C      OBTAIN MODIFIED MATRIX
      CALL REG3
C      OBTAIN INVERSE SOLUTION
      CALL QUAD1(RESULT,IBASIS)
      DO 34 I = 1,LMAX
34  ZP(I) = 0.
      DO 35 I = 1,LMAX
          J = IBASIS(I)
          IF(J.GT.LMAX) GO TO 35
          ZP(J) = RESULT(I)
35  CONTINUE
C      EVALUATE ERROR
      CALL REG4(UAVG)
      DO 24 I = 1,IMAX
C          Z(I) = ORIGINAL DISTRIBUTION
C          ZP(I) = BACK SOLUTION
C          U(I) = CORRESPONDS TO INPUT DATA, COMPUTED USING
C          Z(I)
C          UP(I) = BACK SOLUTION COMPUTATION
C          S(I) = VARIABLE FOR Z(I), CORRESPONDING TO
C          MOLECULAR WEIGHT
      WRITE(6,2001) I,ZP(I),I,Z(I),I,UP(I),I,U(I),I,S(I)
24  CONTINUE
      WRITE(6,2000) (I,ALPHA(I),I = NFIRST,NLAST)
      WRITE(6,2002) UAVG
      WRITE(6,104) XSIG
      WRITE(6,1000)
      GO TO 30
31  READ(5,102) ALPHA(NLAST)
30  CONTINUE
      READ(5,100) IT1,IT2
      IF(IT1.EQ.0) GO TO 99
      GO TO 81
99  CONTINUE
      WRITE(6,1001)
      WRITE(6,7000)
      STOP

```

SECRET

```

43 SIG = 4.
44 COEF = COEF + SIG*XK(I,J)*ZP(J)/(3.*DLS)
41 CONTINUE
   UP(I) = COEF
   UAV = UAV + (UP(I)-U(I))**2
40 CONTINUE
   UAVG = SQRT(UAV/FLOAT(IMAX))
99 RETURN
   END

```

SUBROUTINE REG2

PURPOSE

THIS SUBROUTINE INTEGRATES $XK(I,J)*XK(I,J)$ OVER
ZI-VALUES TO OBTAIN NEW MATRIX $BK(I,J)$

USAGE

CALL REG2

SUBROUTINE REG2

COMMON/ZYT/U,XK,S,X,Z,BK,B,ZP,A,ALPHA,R,XX,UP,DLX,DLS,
*IMAX,NMAX,NF

1IRST,NLAST,FACTO,TCOST,TPIV

DIMENSIONS FOR COMMON

DIMENSION U(60),XK(60,60),S(60),X(60),Z(60),BK(60,60),
*B(60),ZP(60)

```
1,A(60,60),ALPHA(10),R(60),XX(60),UP(60)
```

SIMPSON RULE

```
DO 5 I = 1,NMAX
```

DO 5 J = 1,NMAX

COEF1 = 0.

COEF = 0.

```
DO 20 K = 1,IMAX
```

```
IF(K.EQ.1.OR.K.EQ.IMAX) GO TO 21
```

```
IF(K.EQ.2.OR.K.EQ.IMAX-1) GO TO 23
```

$$KNUM = K/2$$
$$JNUM = (K+1)/2$$

```
IF(JNUM.EQ.KNUM) GO TO 23
```

22 SIG = 2.

GO TO 24

21 SIG = 1.

GO TO 24

23 SIG = 4.

```
24 A1 = SIG*XK(K,I)*XK(K,J)/(3.*DLX)
```

```
IF(I.GT.1) GO TO 7
```

SECRET


```

50 IF(LABEL2.GT.NMAX.OR.LABEL2.LT.1) GO TO 59
   QQ = 0.5*A1*A2*ALPHA(N)*(1.E 03*DLS)**N
   A(LABEL1,LABEL2) = A(LABEL1,LABEL2) + QQ
   GO TO 60
59 IF(LABEL2.GT.NMAX) GO TO 58
   LABEL2 = IABS(LABEL2) + 1
   GO TO 50
58 LABEL2 = 2*NMAX - LABEL2 + 1
   GO TO 50
60 CONTINUE
63 CONTINUE
   RETURN
   END

```

FUNCTION CALC

PURPOSE

THIS FUNCTION SUBROUTINE EVALUATES THE
COEFFICIENTS (BINOMIAL), ETC.
CALLED BY REG3

USAGE

X=CALC(N,K,DLS)

FUNCTION CALC(N,K,DLS)

```

LL = 2*N
L = K - 1
M = N - L
IF(K.EQ.1.OR.K.EQ.N+1) GO TO 10
I1 = 1
I2 = 1
I3 = 1
DO 1 I = 1,L
1 I1 = I1*I
DO 3 I = 1,N
3 I3 = I*I3
DO 2 I = 1,M
2 I2 = I*I2
X1 = I3/(I1*I2)
X2 = (-1.)**K
CALC = X1*X2
GO TO 99
10 IF(K.EQ.1) GO TO 11
   X1 = -1.
   CALC = X1
   GO TO 99

```

```
11 X1 = (-1.)**K
   CALC = X1
99 RETURN
END
```

SUBROUTINE QUAD1

PURPOSE

SUBROUTINES QUAD1 AND QUAD2 SOLVE THE QUADRATIC PROGRAMMING PROBLEM, FIND THE VALUE OF X THAT MAXIMIZES

$$A'X - 1/2 X'B X$$

SUBJECT TO

$$C X \leq D$$

$$X \geq 0$$

USING DANTZIG'S MODIFIED SIMPLEX ALGORITHM
(SEE JOHN C. G. BOOT, QUADRATIC PROGRAMMING, RAND MCNALLY, CHICAGO 1964, PP. 186-196)
QUAD1 DEFINES THE INITIAL SIMPLEX TABLEAU

USAGE

CALL QUAD1

(A,B,C,D,N,K,ROWS,COLS,ABCD,RESULT,ZERO1,BASIS)

DESCRIPTION OF PARAMETERS

- A - INPUT VECTOR OF LENGTH N THAT DEFINES THE LINEAR PART OF THE OBJECTIVE FUNCTION
- B - INPUT MATRIX (N,N) THAT DEFINES THE QUADRATIC PART OF THE OBJECTIVE FUNCTION
- C - INPUT MATRIX (K,N) THAT DEFINES THE LEFT HAND PART OF THE CONSTRAINTS
- D - VECTOR OF LENGTH K THAT DEFINES THE RIGHT HAND SIDE OF THE CONSTRAINTS
- N - NUMBER OF ELEMENTS OF X
- K - NUMBER OF CONSTRAINTS
- ROWS - N+K, THE NUMBER OF ROWS IN THE INITIAL SIMPLEX TABLEAU
- COLS - 2*ROWS+1, THE NUMBER OF COLUMNS IN THE INITIAL SIMPLEX TABLEAU
- ABCA - THE INITIAL SIMPLEX TABLEAU, MATRIX OF SIZE (ROWS,COLS)
- RESULT - VECTOR OF LENGTH ROWS, THAT CONTAINS THE RESULTS OF THE QUADRATIC PROGRAMMING PROBLEM
- BASIS - VECTOR OF LENGTH ROWS, CONTAINING THE LOCATIONS OF THE BASIS VECTORS

THE BASIS VECTORS

```

C
C
C
      SUBROUTINE QUAD1(RESULT,BASIS)
      INTEGER ROWS, COLS, ZERO1, BASIS
      COMMON/ZYT/U, XK, S, X, Z, BK, B, ZP, A, ALPHA, R, XX, UP, DLX, DLS,
      *IMAX, NMAX, NF
      1 FIRST, NLAST, FACTO, TCOST, TPIV
C      DIMENSION FOR COMMON
      DIMENSION U(60), XK(60,60), S(60), X(60), Z(60), BK(60,60),
      *B(60), ZP(60)
      1, A(60,60), ALPHA(10), R(60), XX(60), UP(60)
      COMMON/ZXT/ABCD
      DIMENSION C(2,60), D(2), ABCD(60,121), RESULT(60), ZERO1(1
      *21), BASIS(60
      1), IROW(121)
      LOGICAL NOPIVT
      COMMON/QUAD2C/NOPIVT
      N = NMAX
      K = 1
      ROWS = NMAX + K
      COLS = 2*(NMAX + K) + 1
      DO 57 I = 1, NMAX
      C(1,I) = FACTO/DLS
57 CONTINUE
      D(1) = FACTO
C      N VARIABLES      K CONSTRAINTS
      DO 1 I=1, ROWS
      DO 1 J=1, COLS
      1      ABCD(I,J)=0.0
      DO 2 I=1, N
      DO 2 J=1, N
      2      ABCD(I,J) = -A(I,J)
      DO 3 K1=1, K
      I=N+K1
      ABCD(I,I)=1.0
      DO 3 J=1, N
      3      ABCD(I,J)=C(K1,J)
      DO 4 I=1, N
      J=N+K+I
      4      ABCD(I,J)=1.0
      DO 5 K1=1, K
      J=2*N+K+K1
      DO 5 I=1, N
      5      ABCD(I,J)=-C(K1,I)
      J=COLS
      DO 6 I=1, N
      6      ABCD(I,J) = -B(I)
      DO 7 K1=1, K

```

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```

      I=N+K1
7     ABCD(I,J)=D(K1)
      DO 11 I=1,ROWS
      DO 12 J=1,COLS
12    IROW(J)=ABCD(I,J)
11    CONTINUE
      CALL QUAD2(ROWS,COLS,N,K,RESULT,ZERO1,BASIS,TPIV,TCOST
*)
      RETURN
      END
C     *****
C
C     SUBROUTINE QUAD2
C
C     PURPOSE
C       (SEE QUAD1)
C
C     USAGE
C       CALL QUAD2(ABCD,ROWS,COLS,N,K,RESULT,ZERO1,BASIS)
C
C     DESCRIPTION OF PARAMETERS
C       (SEE QUAD1)
C
C
C     SUBROUTINE QUAD2(ROWS,COLS,N,K,RESULT,ZERO1,BASIS,TPIV
*,TCOST)
      INTEGER COLS,ZERO1,ROWS,BASIS,COLN,PIVROW,PC,PR
      COMMON/ZXT/ABCD
      DIMENSION ABCD(60,121),RESULT(60),ZERO1(121),BASIS(60)
      REAL NUM,MULT
      LOGICAL NOPIVT
      COMMON/QUAD2C/NOPIVT
C     CLEAR ZERO1 VECTOR
      DO 2 I=1,COLS
2     ZERO1(I)=0
C     INSERT (N+K) ONES INTO ZERO1(N+1)
      DO 3 I=1,ROWS
      J=N+I
3     ZERO1(J)=1
C     LOAD N COLUMN NUMBERS FROM VARIABLE V(1) INTO BASIS(1)
      DO 4 I=1,N
4     BASIS(I)=ROWS+I
C     LOAD K COLUMN NUMBERS FROM VARIABLE L(N+1) INTO
C     BASIS(N+1)
      DO 9 I=1,K
      J=N+I
9     BASIS(J)=J
C     ASSUME A NON STANDARD TABLE
17    NONSTD=0

```

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```

C   LOOK AT ZERO1 VECTOR AND DETERMINE FOR A NONSTANDARD
C   TABLE.....
C       1. PC=COLUMN NUMBER OF THE MISSING V VARIABLE
C       2. IV=V COLUMN NUMBER OF THE BASIC PAIR
C       3. IF CONDITION 1 AND 2 ARE PRESENT SET NONSTD=1
C       DO 5 I=1,ROWS
C           J=I+ROWS
C           I1=ZERO1(I)+ZERO1(J)
C           IF (I1-1) 6,5,7
C       5   PC=J
C           NONSTD=1
C           GO TO 5
C       7   IV=J
C           NONSTD=1
C       5   CONTINUE
C   IS THIS A NON STANDARD TABLE
C       IF (NONSTD.EQ.1) GO TO 8
C   SCAN THE BASIS FOR IV,COLUMN NUMBER OF THE LARGEST
C   NEGATIVE V(I) AND DETERMINE PC=COLUMN NUMBER OF L(I) TO
C   BE ADDED TO THE BASIS
C       VNEG=0.0
C       DO 10 I=1,ROWS
C           COLN=BASIS(I)
C           IF (COLN.LE.ROWS) GO TO 10
C           T1=ABCD(I,COLS)
C           IF (T1.GE.VNEG) GO TO 10
C           VNEG=T1
C           IV=COLN
C           PC=COLN-ROWS
C   10   CONTINUE
C   LOOK AT THE V(IV) RATIO AND ALL J(I) RATIOS AND
C   DETERMINE THE VARIABLE HAVING THE SMALLEST NON NEGATIVE
C   VALUE. THIS COLUMN NUMBER IS PR (THE PIVOT ROW), THE
C   VARIABLE TO BE REMOVED
C   8   RATIO=1.0E37
C       NOPIVT=.TRUE.
C       DO 11 I=1,ROWS
C           COLN=BASIS(I)
C           DEN=ABCD(I,PC)
C           NUM=ABCD(I,COLS)
C           IF (ABS(DEN) .LT. TPIV)GO TO 11
C       IF (COLN.LE.ROWS) GO TO 13
C       IF (COLN.NE.IV) GO TO 11
C   13   T1=NUM/DEN
C       NOPIVT=.FALSE.
C       IF (T1.LE.0.0) GO TO 11
C       IF (T1.GE.RATIO) GO TO 11
C       PR=COLN
C       PIVROW=I

```

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```

        RATIO=T1
11      CONTINUE
C      ADD AND DELETE THE PROPER VARIABLES FROM THE BASIS AND
C      ZERO1 VECTORS
        ZERO1(PC)=1
        ZERO1(PR)=0
        BASIS(PIVROW)=PC
        PR=PIVROW
C      NORMALIZE THE PIVOT ROW BY THE PIVOT ELEMENT
        DEN=ABCD(PR,PC)
        DO 14 J=1, COLS
14      ABCD(PR,J)=ABCD(PR,J)/DEN
C      ZERO OUT THE REMAINING ELEMENTS OF THE PIVOT COLUMN
        DO 18 I=1, ROWS
        IF (I.EQ.PR) GO TO 18
        MULT=-ABCD(I,PC)
        IF (MULT.EQ.0.0) GO TO 18
        DO 15 J=1, COLS
15      ABCD(I,J)=ABCD(I,J)+MULT*ABCD(PR,J)
18      CONTINUE
C      ARE ANY OF THE BASIC VALUES STILL NEGATIVE
        DO 16 I=1, ROWS
        IF (ABCD(I, COLS) .LT. -ABS(TCOST)) GO TO 17
16      CONTINUE
C      TRANSFER THE LAST COLUMN TO THE SOLUTION VECTOR
        DO 1 I=1, ROWS
1      RESULT(I)=ABCD(I, COLS)
        RETURN
        END

```

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THIS IS FOR A SYMMETRICAL UNIMODAL MOL. WEIGHT DIST. USIN
G REQUAD
4341 0.00000E 00 1.50000E 05
0.400E-04
0 2 2 0 1.0E 00-1.0E-15 1.0E-18
-09-04
0 0

UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Air Force Materials Laboratory Wright-Patterson AFB, Ohio 45433		2a. REPORT SECURITY CLASSIFICATION Unclassified	
		2b. GROUP	
3. REPORT TITLE EVALUATION OF MOLECULAR WEIGHT FROM EQUILIBRIUM SEDIMENTATION. PART VII; MATHEMATICAL ANALYSIS OF THE REGULARIZATION TECHNIQUE INCORPORATED INTO QUADRATIC PROGRAMING			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) Summary Report (September 1971 to May 1972)			
5. AUTHOR(S) (First name, middle initial, last name) Donald R. Wiff Matatiah T. Gehatia Thomas E. Duvall			
6. REPORT DATE December 1972		7a. TOTAL NO. OF PAGES 54	7b. NO. OF REFS 57
8a. CONTRACT OR GRANT NO.		9a. ORIGINATOR'S REPORT NUMBER(S) AFML-TR-67-121, PART VII	
b. PROJECT NO. 7342			
c. Task No. 734203		9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
d.			
10. DISTRIBUTION STATEMENT Approved for public release; distribution unlimited.			
11. SUPPLEMENTARY NOTES		12. SPONSORING MILITARY ACTIVITY Air Force Materials Laboratory (LNP) Wright-Patterson Air Force Base, Ohio 45433	
13. ABSTRACT <p>The equation relating molecular weight distribution of a polymer to the experimental function of concentration appearing in equilibrium sedimentation with the ultracentrifuge is nonsolvable because it is an Improperly Posed Problem in the Hadamard sense. For a simple distribution this equation has been solved by applying a method of regularization. To solve a nonsymmetrical bimodal and a trimodal distribution, the technique of regularization had to be incorporated into a linear programming. In the current work the regularization technique has been incorporated into quadratic programming. This new combined method proved to be more adequate to solve, also more complex distributions such as tri-, tetra-, and pentamodal. In addition, this technique is cheaper, because it requires less computer time than the regularization incorporated into linear programming.</p>			

DD FORM 1473
1 NOV 65

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14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Ill-Posed Problem Regularization Quadratic Programming Ultracentrifugation Equilibrium Sedimentation Molecular Weight Distribution Integral Equations of the First Kind Numerical Analysis						

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